Melting temperature of screened Wigner crystal on helium films by molecular dynamics

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Using molecular dynamics (MD) simulation, we have calculated the melting temperature of two-dimensional electron systems on 240Å-500Å helium films supported by substrates of dielectric constants $\epsilon_s = 2.2 - 11.9$ at areal densities n varying from 3×10^9 cm^{-2} to 1.3×10^{10} cm^{-2}. Our results are in good agreement with the available theoretical and experimental results.

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At suficiently low densities and temperatures, an electron gas is expected to undergo a phase transition to a lattice (because of the domination of the Coulomb interaction energy over the kinetic energy) which has received the name Wigner crystal[1]. The two-dimensional (2d) Wigner crystal is well established and experimentally it was first observed on liquid helium surface[2] and more recently in semiconductors structures like MOSFET's and heterojunctions[3]. These systems can be used for testing several theoretical predictions in many-body theory, such as phase-transitions of the electron system, metal-insulator transition and now electrons on helium surface are being proposed as a set of strongly interacting quantum bits for quantum computers[4]. Electrons on the surface of bulk helium form a crystal at a temperature $T_m = 2e^2(\pi n)^{1/2}/(\epsilon_{He}+1)\Gamma_m$, which is much higher than the Fermi temperature, $T_F = \pi n\hbar^2/m$ in a density range of $10^5 - 10^9$ cm^{-2} (where n is the electron areal density, ϵ_{He} is the dieletric constant of helium and Γ_m is the plasma parameter in the melting temperature defined as the ratio of potential to kinetic energy). Therefore, such electrons in this regime obey the classical Boltzmann statistics. Experimentally the liquid to solid transition in the bulk takes place for a value of the coupling constant $\Gamma_m = 137 \pm 15$[2] and computer simulations of Kalia *et al.*[5] showed an agreement with the experimental measurements indicating a first-order melting in $\Gamma_m = 118 - 130$.

Superficial electrons on liquid helium films form also a very interesting system to study the many-body properties of 2d screened systems. In this case the screening is provided by the image charges in the substrate beneath the film. The screening effect can drastically change the electron-electron interacting potential going from $1/r$ to $1/r^3$ through varying external parameters such as film thickness and dielectric constant of the substrate. Peeters [6] using a phenomenological approach got a reduction in the phase diagram of this electron system comparing with the bulk case. Saitoh[7] obtained the melting transition in this system using an analytical approximation to the angular frequency of the transverse Wigner phonon combined with the Kosterlitz-Thoules melting criterion. His result is in agreement with the experiment by Jiang *et al.*[9]. Cândido *et al.*[8] studied the thermodynamical, structural and dynamical properties of this two-dimensional electron system by computer simulation. Experimmentally, the melting temperature of the Wigner crystal on thin helium films adsorbed on dielectric substrates was measured by Jiang *et al.*[9] through electron mobility and by Mistura *et al.*[10] using microwave cavity technique.

In this paper, we present an accurate MD calculation for the melting temperature for an electron system over a helium film adsorbed on a dielectric substrate. In Fig. 1 we show schematically the geometrical arrangement of the system considered. The obtained results are directly compared with the available experimental data, of Mistura *et al.*[10] and Jiang *et al.*[9], and the theoretical results of Peeters[6] and Saitoh[7].

We consider a two-dimensional system of electrons on a helium film of thickness d adsorbed on a substrate of dielectric constant ϵ_s, interacting through a screening Coulomb potential[11]. The electron system is immersed in a rigid, uniform, positively charged background to make a neutral charged system. The Hamiltonian for such a system is given by

$$H = \frac{1}{2}m\sum_i v_i^2 + \sum_{i>j} e^2 \left[\frac{1}{r_{ij}} - \frac{\delta}{\sqrt{r_{ij}^2 + (2d)^2}}\right] + U_b, \quad (1)$$

where $\delta = (\epsilon_s - 1)/(\epsilon_s + 1)$ with the dielectric constant of helium approximated by 1 ($\epsilon_{He} = 1.057$) and U_b is the interaction of electrons with the uniform positively charged background.

In this work most of the molecular dynamics calculations were performed on a system of 100 electrons with a few runs of 484 and 784 electrons to study size effect. The finite size effect is investigated by changing the system size and the thermodynamical behavior in an infinite system is derived from their extrapolation. The initial position of the electrons is a triangular lattice which is accomodated in a rectangular box with periodic boundary condictions to eliminate the surface effects. Because of the long range nature of the electron-electron

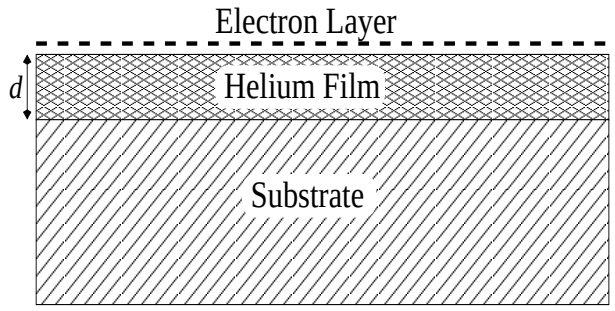

FIG. 1: Schematic view of the electron system.

and electron-background interacting potential we are employing Ewald summation which splits the potential into a long-range and a short-range part. The long-range part is handled in the k-space, while the short range part in the real space. We have used the fifth-order predictor-corrector algoritm to integrate the Newton's equation of motion with the MD time step varying from 10^{-12} to 10^{-15} sec, since it has some scale dependence on the electron densities. The optimum time step leads to a conservation of the total energy of 1 part in 10^4 after several thousand time step runs. The time average of the physical quantities were obtained over 120 000 time steps after the system has reached equilibrium.

In Fig. 2 we present the results for the total energy per electron versus temperature to illustrate the general feature of the melting transition in this system. The solid squares in the figure represent the results for the electron liquid which has been monotonically cooled from a higher temperature. The open circles are the results for the electron solid which has been monotonically heated from a lattice at very low temperatures. It means that our simulations were performed in cascade, i.e., an equilibrated configuration obtained for a given higher (lower) temperature was used as an input to reach another configuration at lower (higher) temperature. As one can see the electron system shows hysteresis and latent heat on melting, which characterize a first order transition as other 2d classical systems. The melting temperature range is 1.83 K $< T <$ 2.05 K defined from the vertical dashed lines in Fig. 2 representing the hysteresis region. Thus, we would define the melting temperature, T_m, as exactly the mean point in the temperature width of the hysteresis ΔT, i.e, $T_m = (1.94 \pm 0.11)$ K with the error bar giving by half the temperature width of the hysteresis. The value of the latent heat per particle and the change in the entropy on melting are found to be 0.40 K and 0.21 k_B, respectively. We also find our MD results for the melting temperature is in agreement with those of Kalia *et al.*[5] for the bulk limit.

Fig. 3 shows size dependences of the transition temperature T_m for different electron densities. The error bars on T_m indicate the hysteresis width. When electron number becomes larger, T_m decreases because the periodic boundary conditions favors the solid phase. The

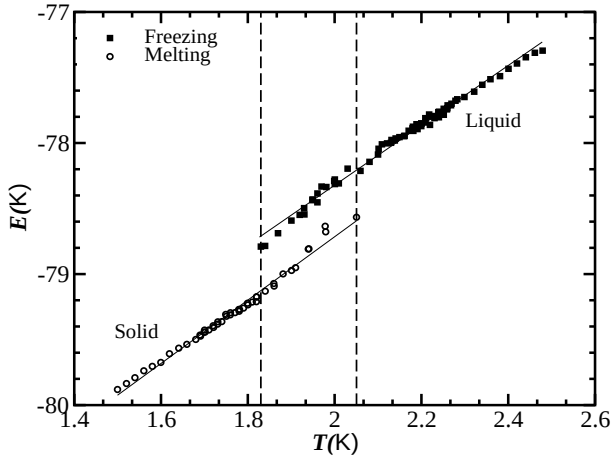

FIG. 2: Total energy per electron as a function of temperature for a system of $N = 100$ electrons on a helium film supported by a glass substrate, $\epsilon_s = 7.3$, film thickness $d = 240$ Å and density $n = 1.3\text{x}10^{10}$ cm^{-2} .

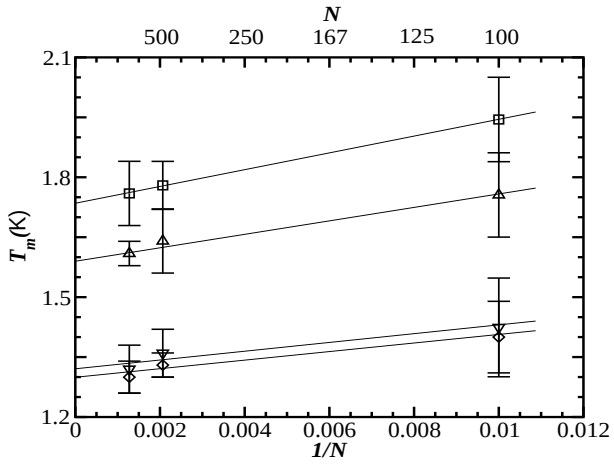

FIG. 3: Size dependence of the melting temperature for electrons on helium films above a substrate with dielectric constant $\epsilon_s = 7.3$ at four different densities: $n = 1.3 \times 10^{10}$ cm^{-2} and $d = 240$ Å(squares); $n = 1.0 \times 10^{10}$ cm^{-2} and $d = 285$ Å(triangles-up); $n = 0.9 \times 10^{10}$ cm^{-2} and $d = 260$ Å(triangles-down); and $n = 0.75 \times 10^{10}$ cm^{-2} and $d = 305$ Å(diamonds). The lines are linear fit.

transition temperature, however, seems to follow a linear decrease as a function of $1/N$. Therefore the melting point in the thermodynamic limit can be obtained definitely by extrapolating the finite size data.

The extrapolated melting temperature is exhibited in Fig. 4 as a function of the electron density (top), film thickness (middle) and dielectric constant of the substrate (bottom). We roughly estimated the error bar on the experimental values for the melting temperature to indicate the uncertainty of about $15\% - 20\%$ on the experimental measurement of the electron density. As is shown in Fig. 4, our results are in good agreement with those obtained experimentally in Ref.[10]. The top panel

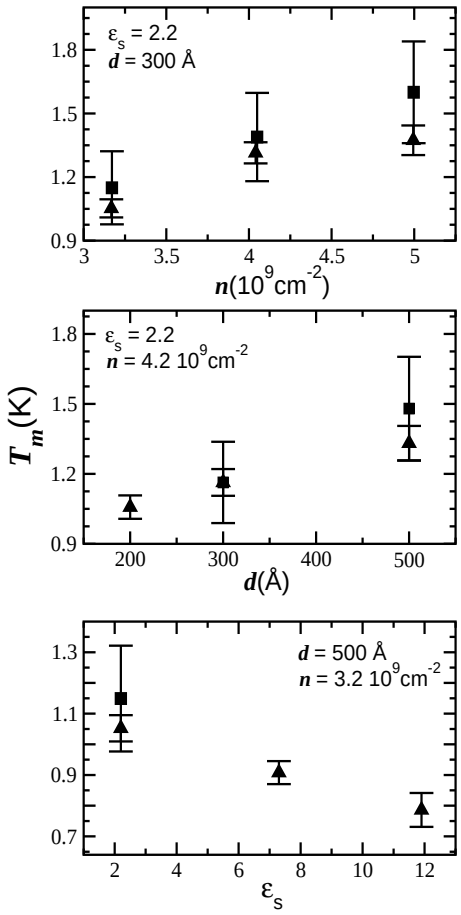

FIG. 4: The melting temperature as a function of the electron density (top), film thickness (middle) and dielectric constant of the substrate (bottom). The experimental results from Ref.[10] are given by solid squares and our MD simulation results are indicated by solid triangles.

shows that the melting temperature increases with increasing the electron density (for fixed ϵ_s and d) due to the the fact that the screening becomes weaker and, consequently, the electron-electron interaction is enhanced. The middle panel also shows a shift in the melting transition to higher temperature with increasing the film thickness (for fixed n and ϵ_s), which is a consequence of decreasing in the screening resulting in a stronger electron-electron interaction. In the bottom panel, the melting temperature decreases as the dielectric constant of the substrate increases at fixed d and n. A larger dielectric constant of the substrate leads to a more polarizable system with stronger screening. As a consequence, the melting temperature goes down.

In table I, we show a comparison of our MD simulation results of the melting temperature with the available theoretical and experimental results for electron systems on a thin helium film surface. For densities below 1.0×10^{10} cm^{-2} one can see that our MD calculations are in agreement with both Jiang *et al.* [9] and Mistura *et al.* [10] experimental measurements. They are also in agreement with Saitoh's theoretical results[7] in the range of the densities studied. However, we got some discrepancies with Peeters's results[6] that can be justified, as pointed out by Saitoh[7], as being a possible double counting on T_m. For densities larger than 1.0×10^{10} cm^{-2}, our MD simulation melting temperatures are higher than the experimental ones, though the differences are almost within the uncertainty of the experimental results. A possible explanation for this discrepancy is that the quantum effect can be important at such densities. Besides, we note that the change in entropy on melting decreases as the density or the dielectric constant of the substrate (the film thichness) increases (decreases). This might imply that transition becomes continuous at high densities.

In conclusion, we have shown that the MD is able to reproduce the experimental measurements of the melting temperature in the two-dimensional electrons on thin liquid He films. Our results are in good agreement with those obtained by Mistura *et al.*[10] and Jiang *et al.*[9]. These results in the classical regime (*i.e.* $n \leq 1.0 \times 10^{10}$ cm^{-2}) should be useful to the experimental and theoretical investigation of the melting transition in this system. For larger densities ($n > 1.0 \times 10^{10}$ cm^{-2} and $\epsilon_s > 2.2$), the results might be beyond the applicability of the present method.

Acknowledgments

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TABLE I: Data of melting temperature T_m for different thicknesses d, dielectric constant of the substrates ϵ_s and electron densities n. The experimental uncertainty in the absolute value of the electron density is about $15\% - 20\%$ in Refs.[9] and [10]. Quantities in ( ) are the estimated error on T_m defined as half of temperature width of the hysteresis, in the last decimal place.

ϵ_s	d(Å)	n (10^{10}cm^{-2})	T_m(K)				
			Mistura et al.[10]	Jiang *et al.*[9]	Peeters[6]	Saitoh[7]	MD - this work
2.2	300	0.42	1.16	–	–	1.08	1.16(6)
2.2	300	0.53	1.43	–	–	1.21	1.26(7)
2.2	300	0.57	1.50	–	–	1.26	1.33(6)
2.2	500	0.32	1.15	–	–	1.05	1.05(4)
2.2	500	0.40	1.39	–	–	1.17	1.31(5)
2.2	500	0.50	1.60	–	–	1.29	1.37(7)
3.9	237	1.05	1.16	–	–	–	1.64(9)
7.3	305	0.75	–	1.23	0.85	1.24	1.29(5)
7.3	260	0.90	–	1.28	0.89	1.31	1.32(8)
7.3	285	1.00	–	1.32	1.02	1.54	1.59(7)
7.3	240	1.30	–	1.38	1.14	1.62	1.73(8)

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